Dmitry A Filimonov

List of Publications by Year
in descending order

96 papers	5,746 citations	126708 33 h-index	82410 72 g-index
106 all docs	106 docs citations	106 times ranked	4631 citing authors

#	Article	IF	Citations
1	PASS: prediction of activity spectra for biologically active substances. Bioinformatics, 2000, 16, 747-748.	1.8	737
2	Prediction of the Biological Activity Spectra of Organic Compounds Using the Pass Online Web Resource. Chemistry of Heterocyclic Compounds, 2014, 50, 444-457.	0.6	630
3	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
4	QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction. Molecular Informatics, 2011, 30, 241-250.	1.4	278
5	Robustness of Biological Activity Spectra Predicting by Computer Program PASS for Noncongeneric Sets of Chemical Compounds. Journal of Chemical Information and Computer Sciences, 2000, 40, 1349-1355.	2.8	217
6	PASS Biological Activity Spectrum Predictions in the Enhanced Open NCI Database Browser. Journal of Chemical Information and Computer Sciences, 2003, 43, 228-236.	2.8	203
7	Chemical Similarity Assessment through Multilevel Neighborhoods of Atoms:â€‰ Definition and Comparison with the Other Descriptors. Journal of Chemical Information and Computer Sciences, 1999, 39, 666-670.	2.8	192
8	Computer-Aided Discovery of Anti-Inflammatory Thiazolidinones with Dual Cyclooxygenase/Lipoxygenase Inhibition. Journal of Medicinal Chemistry, 2008, 51, 1601-1609.	2.9	161
9	Multi-Targeted Natural Products Evaluation Based on Biological Activity Prediction with PASS. Current Pharmaceutical Design, 2010, 16, 1703-1717.	0.9	126
10	Discriminating between Drugs and Nondrugs by Prediction of Activity Spectra for Substances (PASS). Journal of Medicinal Chemistry, 2001, 44, 2432-2437.	2.9	124
11	Prediction of Biological Activity Spectra for Substances: Evaluation on the Diverse Sets of Drug-Like Structures. Current Medicinal Chemistry, 2003, 10, 225-233.	1.2	117
12	CLC-Pred: A freely available web-service for in silico prediction of human cell line cytotoxicity for drug-like compounds. PLoS ONE, 2018, 13, e0191838.	1.1	116
13	Design, synthesis, computational and biological evaluation of new anxiolytics. Bioorganic and Medicinal Chemistry, 2004, 12, 6559-6568.	1.4	114
14	Computer-aided prediction of biological activity spectra for chemical compounds: opportunities and limitation. Biomedical Chemistry Research and Methods, 2018, 1, e00004.	0.1	99
15	PASS: identification of probable targets and mechanisms of toxicity. SAR and QSAR in Environmental Research, 2007, 18, 101-110.	1.0	95
16	Collaborative development of predictive toxicology applications. Journal of Cheminformatics, 2010, 2, 7.	2.8	91
17	DIGEP-Pred: web service for in silico prediction of drug-induced gene expression profiles based on structural formula. Bioinformatics, 2013, 29, 2062-2063.	1.8	87
18	QNA-based â€˜Star Trackâ€™ QSAR approach. SAR and QSAR in Environmental Research, 2009, 20, 679-709.	1.0	84

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19	How to acquire new biological activities in old compounds by computer prediction. Journal of Computer-Aided Molecular Design, 2002, 16, 819-824.	1.3	83
20	SOMP: web server for in silico prediction of sites of metabolism for drug-like compounds. Bioinformatics, 2015, 31, 2046-2048.	1.8	83
21	Design of New Cognition Enhancers:â€‰ From Computer Prediction to Synthesis and Biological Evaluation. Journal of Medicinal Chemistry, 2004, 47, 2870-2876.	2.9	75
22	Fragment-based design, docking, synthesis, biological evaluation and structureâ€“activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as cycloxygenase/lipoxygenase inhibitors. European Journal of Medicinal Chemistry, 2012, 47, 111-124.	2.6	72
23	Quantitative Prediction of Antitarget Interaction Profiles for Chemical Compounds. Chemical Research in Toxicology, 2012, 25, 2378-2385.	1.7	70
24	Probabilistic Approaches in Activity Prediction. , 2008, , 182-216.		67
25	Prediction of Biological Activity Spectra via The Internet. SAR and QSAR in Environmental Research, 2003, 14, 339-347.	1.0	56
26	PASS Targets: Ligand-based multi-target computational system based on a public data and naÃ¯ve Bayes approach. SAR and QSAR in Environmental Research, 2015, 26, 783-793.	1.0	52
27	Top 200 Medicines: Can New Actions be Discovered Through Computer-aided Prediction?. SAR and QSAR in Environmental Research, 2001, 12, 327-344.	1.0	50
28	Metabolism Site Prediction Based on Xenobiotic Structural Formulas and PASS Prediction Algorithm. Journal of Chemical Information and Modeling, 2014, 54, 498-507.	2.5	50
29	MetaTox: Web Application for Predicting Structure and Toxicity of Xenobioticsâ€™ Metabolites. Journal of Chemical Information and Modeling, 2017, 57, 638-642.	2.5	50
30	ADVERPredâ€“Web Service for Prediction of Adverse Effects of Drugs. Journal of Chemical Information and Modeling, 2018, 58, 8-11.	2.5	50
31	A new approach to QSAR modelling of acute toxicityâ€. SAR and QSAR in Environmental Research, 2007, 18, 285-298.	1.0	49
32	Computerâ€Aided Prediction of Rodent Carcinogenicity by PASS and CISOCâ€PSCT. QSAR and Combinatorial Science, 2009, 28, 806-810.	1.5	43
33	Computer-Aided Selection of Potential Antihypertensive Compounds with Dual Mechanism of Action. Journal of Medicinal Chemistry, 2003, 46, 3326-3332.	2.9	40
34	Predicting Biotransformation Potential from Molecular Structure. Journal of Chemical Information and Computer Sciences, 2003, 43, 1636-1646.	2.8	40
35	Directions in QSAR Modeling for Regulatory Uses in OECD Member Countries, EU and in Russia. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2008, 26, 201-236.	2.9	35
36	QSAR Modeling Using Large-Scale Databases: Case Study for HIV-1 Reverse Transcriptase Inhibitors. Journal of Chemical Information and Modeling, 2015, 55, 1388-1399.	2.5	34

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37	A New Statistical Approach to Predicting Aromatic Hydroxylation Sites. Comparison with Model-Based Approaches. Journal of Chemical Information and Computer Sciences, 2004, 44, 1998-2009.	2.8	31
38	Rational Design of Macrolides by Virtual Screening of Combinatorial Libraries Generated through in Silico Manipulation of Polyketide Synthases. Journal of Medicinal Chemistry, 2006, 49, 2077-2087.	2.9	28
39	Computer-aided prediction of QT-prolongation. SAR and QSAR in Environmental Research, 2008, 19, 81-90.	1.0	27
40	How to Achieve Better Results Using PASS-Based Virtual Screening: Case Study for Kinase Inhibitors. Frontiers in Chemistry, 2018, 6, 133.	1.8	27
41	A Computational Approach for the Prediction of HIV Resistance Based on Amino Acid and Nucleotide Descriptors. Molecules, 2018, 23, 2751.	1.7	25
42	Prediction of reacting atoms for the major biotransformation reactions of organic xenobiotics. Journal of Cheminformatics, 2016, 8, 68.	2.8	24
43	ROSC-Pred: web-service for rodent organ-specific carcinogenicity prediction. Bioinformatics, 2018, 34, 710-712.	1.8	24
44	AntiBac-Pred: A Web Application for Predicting Antibacterial Activity of Chemical Compounds. Journal of Chemical Information and Modeling, 2019, 59, 4513-4518.	2.5	24
45	Computer-aided prediction of xenobiotic metabolism in the human body. Russian Chemical Reviews, 2016, 85, 854-879.	2.5	22
46	Online resources for the prediction of biological activity of organic compounds. Russian Chemical Bulletin, 2016, 65, 384-393.	0.4	22
47	Computer-aided rodent carcinogenicity prediction. Mutation Research - Genetic Toxicology and Environmental Mutagenesis, 2005, 586, 138-146.	0.9	21
48	Drug-drug interaction prediction using PASS. SAR and QSAR in Environmental Research, 2019, 30, 655-664.	1.0	19
49	Prediction of Proteinâ€“Ligand Interaction Based on the Positional Similarity Scores Derived from Amino Acid Sequences. International Journal of Molecular Sciences, 2020, 21, 24.	1.8	19
50	Web Resources for Discovery and Development of New Medicines. Pharmaceutical Chemistry Journal, 2017, 51, 91-99.	0.3	18
51	Computer aided prediction of biological activity spectra: Evaluating versus known and predicting of new activities for thiazole derivatives. SAR and QSAR in Environmental Research, 2002, 13, 457-471.	1.0	17
52	Why relevant chemical information cannot be exchanged without disclosing structures. Journal of Computer-Aided Molecular Design, 2005, 19, 705-713.	1.3	17
53	Prediction of biological activity profiles of cyanobacterial secondary metabolites. SAR and QSAR in Environmental Research, 2007, 18, 629-643.	1.0	17
54	Design, Synthesis and Pharmacological Evaluation of Novel Vanadium-Containing Complexes as Antidiabetic Agents. PLoS ONE, 2014, 9, e100386.	1.1	17

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55	Comparison of Quantitative and Qualitative (Q)SAR Models Created for the Prediction of Ki and IC50 Values of Antitarget Inhibitors. Frontiers in Pharmacology, 2018, 9, 1136.	1.6	17
56	Computer-Aided Estimation of Biological Activity Profiles of Drug-Like Compounds Taking into Account Their Metabolism in Human Body. International Journal of Molecular Sciences, 2020, 21, 7492.	1.8	17
57	Prediction and Study of Anticonvulsant Properties of Benzimidazole Derivatives. Pharmaceutical Chemistry Journal, 2017, 50, 775-780.	0.3	16
58	Data Mining Approach for Extraction of Useful Information About Biologically Active Compounds from Publications. Journal of Chemical Information and Modeling, 2019, 59, 3635-3644.	2.5	16
59	Combined network pharmacology and virtual reverse pharmacology approaches for identification of potential targets to treat vascular dementia. Scientific Reports, 2020, 10, 257.	1.6	16
60	PASS-based approach to predict HIV-1 reverse transcriptase resistance. Journal of Bioinformatics and Computational Biology, 2017, 15, 1650040.	0.3	15
61	Prediction of Severity of Drug-Drug Interactions Caused by Enzyme Inhibition and Activation. Molecules, 2019, 24, 3955.	1.7	15
62	Antihypoxic Action of Panax Japonicus, Tribulus Terrestris and Dioscorea Deltoidea Cell Cultures: In Silico and Animal Studies. Molecular Informatics, 2020, 39, e2000093.	1.4	15
63	Prediction of Drug-Drug Interactions Related to Inhibition or Induction of Drug-Metabolizing Enzymes. Current Topics in Medicinal Chemistry, 2019, 19, 319-336.	1.0	15
64	Functional classification of proteins based on projection of amino acid sequences: application for prediction of protein kinase substrates. BMC Bioinformatics, 2010, 11, 313.	1.2	14
65	Identification of Drug-Induced Myocardial Infarction-Related Protein Targets through the Prediction of Drugâ€“Target Interactions and Analysis of Biological Processes. Chemical Research in Toxicology, 2014, 27, 1263-1281.	1.7	14
66	Metatox - Web application for generation of metabolic pathways and toxicity estimation. Journal of Bioinformatics and Computational Biology, 2019, 17, 1940001.	0.3	13
67	A Computational Approach for the Prediction of Treatment History and the Effectiveness or Failure of Antiretroviral Therapy. International Journal of Molecular Sciences, 2020, 21, 748.	1.8	13
68	In silicomethod for identification of promising anticancer drug targets. SAR and QSAR in Environmental Research, 2009, 20, 755-766.	1.0	12
69	In Silico Identification of Proteins Associated with Drug-induced Liver Injury Based on the Prediction of Drug-target Interactions. Molecular Informatics, 2017, 36, 1600142.	1.4	12
70	Prediction of metabolites of epoxidation reaction in MetaTox. SAR and QSAR in Environmental Research, 2017, 28, 833-842.	1.0	12
71	Data and Text Mining Help Identify Key Proteins Involved in the Molecular Mechanisms Shared by SARS-CoV-2 and HIV-1. Molecules, 2020, 25, 2944.	1.7	12
72	Identification of Drug Targets Related to the Induction of Ventricular Tachyarrhythmia Through a Systems Chemical Biology Approach. Toxicological Sciences, 2015, 145, 321-336.	1.4	11

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73	Nootropic action of some antihypertensive drugs: computer predicting and experimental testing. Pharmaceutical Chemistry Journal, 2012, 45, 605-611.	0.3	10
74	PASS-based prediction of metabolites detection in biological systems. SAR and QSAR in Environmental Research, 2019, 30, 751-758.	1.0	10
75	Prediction of Protein Functional Specificity without an Alignment. OMICS A Journal of Integrative Biology, 2006, 10, 56-65.	1.0	9
76	AntiHIV-Pred: web-resource for in silico prediction of anti-HIV/AIDS activity. Bioinformatics, 2020, 36, 978-979.	1.8	9
77	In Silico Prediction of Drugâ€“Drug Interactions Mediated by Cytochrome P450 Isoforms. Pharmaceutics, 2021, 13, 538.	2.0	9
78	RECOGNITION OF PROTEIN FUNCTION USING THE LOCAL SIMILARITY. Journal of Bioinformatics and Computational Biology, 2008, 06, 709-725.	0.3	8
79	QNA-Based Prediction of Sites of Metabolism. Molecules, 2017, 22, 2123.	1.7	8
80	Integral estimation of xenobioticsâ€™ toxicity with regard to their metabolism in human organism. Pure and Applied Chemistry, 2017, 89, 1449-1458.	0.9	8
81	Computer-aided prediction of receptor profile for drug-like compounds. SAR and QSAR in Environmental Research, 2002, 13, 433-444.	1.0	7
82	In Silico fragment-based drug design using a PASS approach. SAR and QSAR in Environmental Research, 2012, 23, 279-296.	1.0	7
83	Assessment of the cardiovascular adverse effects of drug-drug interactions through a combined analysis of spontaneous reports and predicted drug-target interactions. PLoS Computational Biology, 2019, 15, e1006851.	1.5	7
84	Extraction of Data on Parent Compounds and Their Metabolites from Texts of Scientific Abstracts. Journal of Chemical Information and Modeling, 2021, 61, 1683-1690.	2.5	7
85	(Q)SAR Models of HIV-1 Protein Inhibition by Drug-Like Compounds. Molecules, 2020, 25, 87.	1.7	6
86	Prediction of Proteinâ€“ligand Interaction Based on Sequence Similarity and Ligand Structural Features. International Journal of Molecular Sciences, 2020, 21, 8152.	1.8	6
87	Computer-Aided Estimation of Synthetic CompoundsSimilarity with Endogenous Bioregulations. QSAR and Combinatorial Science, 1998, 17, 459-464.	1.4	6
88	Prediction of amino acid positions specific for functional groups in a protein family based on local sequence similarity. Journal of Molecular Recognition, 2016, 29, 159-169.	1.1	5
89	MetaPASS: A Web Application for Analyzing the Biological Activity Spectrum of Organic Compounds Taking into Account their Biotransformation. Molecular Informatics, 2021, 40, 2000231.	1.4	5
90	Relationships between the Structure and Severe Drug-Induced Liver Injury for Low, Medium, and High Doses of Drugs. Chemical Research in Toxicology, 2022, 35, 402-411.	1.7	4

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91	The method predicting interaction between protein targets and small-molecular ligands with the wide applicability domain. Computational Biology and Chemistry, 2022, 98, 107674.	1.1	4
92	Virtual Screening for Potential Substances for the Prophylaxis of HIV Infection in Libraries of Commercially Available Organic Compounds. Pharmaceutical Chemistry Journal, 2013, 47, 343-360.	0.3	3
93	In silico assessment of acute toxicity in rodents. Toxicology Letters, 2009, 189, S264.	0.4	2
94	Capacities of computer evaluation of hidden potential of phytochemicals of medicinal plants of the traditional Indian Ayurvedic medicine. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2016, 10, 43-54.	0.2	2
95	Improving (Q)SAR predictions by examining bias in the selection of compounds for experimental testing. SAR and QSAR in Environmental Research, 2019, 30, 759-773.	1.0	2
96	Computer prediction of biological activity spectra for low-molecular peptides and peptidomimetics. Russian Journal of Bioorganic Chemistry, 2000, 26, 297-305.	0.3	1